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TITLE: Excited states of an F'-center

SOURCE: Kishinev. Universitet. Uchenyye zapiski. v. 49, 1961, 19-25

TEXT: The author continues previous work (Uch. zap. KGU 55, 183, 1960) in which he studied the photo-ionization of an F'-center. Here the excited spectrum of an F' center is calculated and the polaron wave function of this spectrum is derived more exactly than before. The Hamiltonian of the crystal in effective-mass representation

$$\hat{H}=-\frac{\hbar^2}{2\mu}(\Delta_1+\Delta_2)+u_1(r_1)+u_2(r_2)+u_{12}(r_{12})+\sum_x A_x(r_1)q_x+$$
$$+\sum_x A_x(r_2)q_x+\frac{\hbar\omega}{2}\sum_x\left(q_x^2-\frac{\partial^2}{\partial q_x^2}\right), \quad (1)$$

and the approximate wave function of the ground state, rewritten in variables of the polaron theory

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$$\Psi_{s,\ldots,n_x}(\vec{r}_1,\vec{r}_2,\xi q)=\Psi_{F'}(r_1)\Psi_{F'}(r_2)\varphi_s(\xi)\prod_x{}'\Phi_{n_x}(q_x-r_{xF'}). \quad (2)$$

(cf. ZhETF, 21, 11, 1951), are used to investigate the state of an F' center in which one of the electrons is excited. $\Psi_{F'}(r)$ is the wave function of an electron localized in an F' center and $\varphi_s(\xi)$ is an approximate wave function, determined from the variation of

$$\overline{H}_s=\int\varphi_s^*(\xi)\left[-\frac{\hbar^2}{2M_0}\Delta_\xi+\frac{\hbar\omega}{2}\sum_x(q_{x\xi}-q_{x0})^2\right]\varphi_s(\xi)\,d\tau_\xi. \quad (3);$$

M_0 is the polaron effective mass and Φ_{n_x} are the wave functions of the harmonic oscillators of the lattice.

$$\hat{W}(r_1, r_2, q) = U_1(r_1) + U_{12}(r_{12}) + \sum_x A_x(r_1)(q_x - q_{x\xi}) + \sum_x A_x(r_2)(q_x - q_{x_F}). \quad (6)$$

is taken as a perturbation operator. $q_{x\xi}$ is the displacement of the equilibrium position of lattice oscillators, caused by an electron localized in the polarization potential well of a polaron, and q_{x_0} is that caused by an electron localized in the F' center. In zeroth approximation

$$\Psi^0_\kappa(r_1, r_2) = \Psi_0(|\vec{r_1} - \vec{\xi}|)\Psi_F(r_2), \quad (10),$$

where Ψ_0 and Ψ_F are the wave functions of electrons localized respectively in the polaron and in F-center potential wells. These functions are

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considered as normalized ones. For the adiabatic potential

$$F(q) = I_1 + I_2 - ce^2 \int \frac{\psi_0^2(|\vec{r_1} - \vec{\xi}|)\,\psi_F^2(r_2)}{|\vec{r_1} - \vec{r_2}|} d\tau_1 d\tau_2 + \frac{\hbar\omega}{2}\sum_{xj}(q_x - q_{x\kappa})^2; \quad (16)$$

is obtained; I_1 and I_2 are the adiabatic potentials of F-center and polaron. From the Schrödinger equation

$$-\frac{\hbar^2}{2M_0}\Delta_\xi \varphi_\kappa(\xi) + K(\xi)\varphi_\kappa(\xi) = E_{s,\ldots n_x \ldots \kappa}\varphi_\kappa(\xi) \quad (23)$$

whose solution is the polaron wave function $\varphi_\kappa(\xi)$ and whose potential is given by

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$$K(\xi) = -\frac{e^2(3\gamma^2-1)}{\varepsilon(\gamma^2-1)^3}\left(e^{-2\gamma\alpha_0\xi}-e^{-2\alpha_0\xi}\right)- \\ -\frac{e^2\alpha_0}{\varepsilon(\gamma^2-1)^2}\left[\gamma e^{-2\gamma\alpha_0\xi}+(2\gamma^2-1)e^{-2\alpha_0\xi}\right], \quad (25)$$

$$\gamma = 1+\frac{16}{5\varepsilon c}. \quad (26),$$

the discrete level of the polaron ground state is calculated, i. e. the variation of $E(\beta)$ is determined:

$$E(\beta) = \int \varphi_\kappa^*(\xi)\left[-\frac{\hbar^2}{2M_0}\Delta_\xi + K(\xi\gamma)\right]\varphi_\kappa(\xi)d\tau_\xi = min, \quad (28)$$

$$\frac{E(\beta)}{A} = \beta^2 - 2A_1\beta^3\left[\frac{1}{(\alpha_1\gamma+\beta)^2}-\frac{1}{(\alpha_1+\beta)^2}\right]-\frac{2B\beta^3}{(\alpha_1+\beta)^3}-\frac{2C\beta^3}{(\alpha_1\gamma+\beta)^3}, \quad (29)$$

$$A_1 = \frac{(3\gamma^2-1)\alpha_1}{(\gamma^2-1)^3};\quad B = \frac{\alpha_1^2(2\gamma^2-1)}{(\gamma^2-1)^2};\quad C = \frac{\alpha_1^2\gamma}{(\gamma^2-1)^3}; \quad (30)$$

$$A = \frac{M_0e^4}{2\hbar^2\varepsilon^2};\quad \alpha_1 = \frac{5}{16}\frac{\mu}{M_0}\varepsilon c. \quad (31)$$

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$$\varphi_0(\xi) = \frac{\beta^{3/2}}{\sqrt{\pi}}exp(-\beta\xi). \quad (27).$$

(29) is minimized numerically for NaCl (β/α_0=3.4), KCl (3.0) and KBr (2.7) and for E_1 -0.053, -0.029 and -0.021 ev is obtained. For the potential energy

$$K(\xi) = \begin{cases} -|K(0) & \text{при } \xi\leqslant\xi_0 \\ 0 & \text{при } \xi>\xi_0, \end{cases} \quad (32)$$

$$K(0) = \frac{5}{8}A\varepsilon c\,\frac{(2\gamma^3-3\gamma^2+1)}{(\gamma-1)(\gamma^2-1)^2}, \quad (33)$$

$$A = \frac{\mu e^4}{2\hbar^2\varepsilon^2}. \quad (34)$$

with ξ_0 = 0.32 Å (NaCl), 0.44 Å (KCl) and 0.73 Å (KBr) the following

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is obtained: $K(0) = -0.11$ ev (NaCl), -0.058 ev (KCl) and -0.051 ev (KBr). For the continuous spectrum of a polaron in a square potential well $K_o^2 = K^2 + \frac{2M_o}{\hbar^2}|K(0)|$ for $\xi < \xi_o$ and $K = (2E_e M_o/\hbar)^{1/2}$ for $\xi > \xi_o$. There are 2 tables.